## 1,5,7,11-Tetraoxaspiro[5.5]undecane 24472-02-4 | DTXSID1066994

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## **Model Performance**

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N	Model	Data	

# Weighted KNN model

5-fold CV (	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

## Model Results

Predicted value: 2.73

Global applicability domain: Inside

Local applicability domain index: 5.29e-01

Confidence level: 7.10e-01

## Nearest Neighbors from the Training Set

Image not found

Dimethoate
Measured: 1.58
Predicted: 1.88

Image not found

2-Isopropyl-6-methyl-4-

pyrimidone Measured: 1.82 Predicted: 2.23 Image not found

Paraldehyde Measured: 3.02 Predicted: 2.77

Image not found

Bromacil Measured: 3.24 Predicted: 2.87 Image not found

4-Methylimidazolidine-2-thione

Measured: 10.0 Predicted: 4.59